N,N,N',N',N",N"-Hexakis(methoxymethyl)-1,3,5-triazine-2,4,6-triamine
3089-11-0 | DTXSID9027520

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 11.7

Global applicability domain: Inside

Local applicability domain index: 6.27e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

Image not found
Octachlorodibenzofuran
Measured: 11.9
Predicted: 11.7

Image not found
Octachlorodibenzo-p-dioxin
Measured: 12.1
Predicted: 11.6

Image not found
2,2',4,4',5-Pentabromodiphenyl
ether
Measured: 11.3
Predicted: 11.5

Image not found
2,2',3,4,4'-Pentabromodiphenyl
ether (BDE 85)
Measured: 11.7
Predicted: 11.5

Image not found
1,2,3,4,7,8,9-
Heptachlorodibenzofuran
Measured: 11.4
Predicted: 10.9